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Discretization of Layer Potentials and Numerical Methods for Water Waves

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It is a pleasure to take part in this remembrance of Professor Tosio Kato. His work was very influential for mathematicians of my generation who were interested in mathematical analysis related to physical problems. I first benefited from his point of view when I studied his book *Perturbation Theory for Linear Operators* as a graduate student. I believe that the high degree of maturity and special care with writing in this book, and in his papers, made his work especially valuable for others to learn from.

We are concerned here with the calculation of singular, or nearly singular, integrals and applications to numerical methods for time-dependent fluid flow. Mathematical models of many problems in science can be formulated in terms of singular integrals. The most familiar case is the use of single or double layer potentials to represent solutions of Laplace's equation. Numerical methods for solving various problems could be based on integral formulations. Thus there is a need for accurate and efficient numerical methods for calculating such integrals. We will describe one approach, in which we replace the singularity with a regularized version, compute a sum in a standard way, and then add corrections which are found by asymptotic analysis near the singularity. We have used this approach to design a convergent numerical method for three-dimensional water waves, based on boundary integrals [4]. The choice of the discretization of the boundary integrals affects the numerical stability of the method. The stability analysis involves considerations very close to the study of linear evolution equations, and the point of view of linear operators is helpful. In this work the sums replacing the layer potentials are treated as discrete versions of pseudodifferential operators. In related work [7] with M.-C. Lai we have developed techniques for computing nearly singular integrals, such as a double layer potential on a curve in the plane at a point near the curve. This technique can be used, for example, to solve a Dirichlet problem at grid points inside the curve without having to discretize the enclosed region.

1. Quadrature of singular integrals. Let us recall first that a single layer potential

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on a surface $S \subseteq \mathbf{R}^3$ has the form

$$u(x) = \int_S G(x-y) \sigma(y) dS(y) \quad (1)$$

for some function σ on S . Here $G(x)$ is the fundamental solution or Green's function for the Laplace operator on \mathbf{R}^3 , $G(x) = -1/4\pi|x|$. It is well known that $\Delta u = 0$ on $\mathbf{R}^3 - S$, and u is continuous across S , but $\partial u / \partial n$ has a jump at S . Similarly, the double layer potential is defined as

$$v(x) = \int_S \frac{\partial G(x-y)}{\partial n(y)} \mu(y) dS(y) \quad (2)$$

where $n(y)$ is the normal vector. We will be concerned with finding discrete approximations to single layer potentials using values at points which are regularly spaced in some coordinate system.

For a smooth integrand, an integral is well approximated by a sum with equal weights. Suppose $f : \mathbf{R}^d \rightarrow \mathbf{R}$ is smooth and rapidly decreasing. We can approximate the integral I with the sum S ,

$$I = \int_{\mathbf{R}^d} f(x) dx, \quad S = \sum_{j \in \mathbf{Z}^d} f(jh) h^d. \quad (3)$$

Here j is a d -tuple of integers and $h > 0$ is the mesh size. The sum is a high order approximation; specifically, for $\ell \geq d+1$,

$$|S - I| \leq C_\ell h^\ell \|D^\ell f\|_{L^1} \quad (4)$$

where ℓ can be large depending on the smoothness of f . This fact can be seen from the Poisson Summation Formula (see [1])

$$(2\pi)^{-d/2} \sum_{j \in \mathbf{Z}^d} f(jh) h^d = \sum_{k \in \mathbf{Z}^d} \hat{f}(2\pi k/h) \quad (5)$$

where \hat{f} is the Fourier transform

$$\hat{f}(k) = (2\pi)^{-d/2} \int_{\mathbf{R}^d} f(x) e^{-ikx} dx. \quad (6)$$

When the integrand is singular, however, the situation is very different. As a simple example, we compare

$$I = \int_{\mathbf{R}^2} \frac{f(x)}{|x|} dx, \quad S = \sum_{j \neq 0} \frac{f(jh)}{|jh|} h^2 \quad (7)$$

where again f is smooth and rapidly decreasing. (We can think of this as a special case of the single layer potential where the surface S is flat.) In this case the error is $O(h)$;

it goes to zero as $h \rightarrow 0$, but not very fast. Fortunately, we know the form of the error more precisely:

$$I = S + c_0 f(0)h + O(h^3) \quad (8)$$

where c_0 is a particular constant, $c_0 \approx 3.900265$. Thus we can correct the sum so that the error is $O(h^3)$, a great improvement. The derivation of this fact can be found in [8]; there is an interesting connection with number theory. This fact is useful once known, but such constants are difficult to find. They also depend on the singularity. If instead of $1/|x|$ we had $1/\sqrt{q(x)}$ with $q(x) = g_{11}x_1^2 + 2g_{12}x_1x_2 + g_{22}x_2^2$, the error would be qualitatively similar, but the constant c_0 would depend on g_{ij} .

The example above illustrates a general principle about quadrature (or discrete approximation) of singular integrals. We will consider an integrand of the form $K(x)f(x)$, with $x \in \mathbb{R}^d$, where K is smooth for $x \neq 0$ and homogeneous of degree m ; that is, for $a > 0$, $K(ax) = a^m K(x)$. (In our example, $m = -1$.) We also assume f is smooth and rapidly decreasing, and $m \geq 1 - d$. We now compare

$$I = \int_{\mathbb{R}^d} K(x)f(x) dx, \quad S = \sum_{j \neq 0} K(jh)f(jh) h^d \quad (9)$$

where $j \in \mathbb{Z}^d$. Then

$$S - I = h^{d+m}(c_0 f(0) + C_1 h + C_2 h^2 + \dots) \quad (10)$$

Here c_0 depends only on K , but C_k depends on f as well. This fact was derived in [14]; a nice proof was given in [9] which can be adapted to different cases. If c_0 is known, the leading error can be subtracted out, but again it is difficult to find. Sometimes $C_1 = 0$ by symmetry; this was the case in the example.

Our approach is to use regularly spaced points, as above, but to replace the singular kernel $K(x)$ with regularized, or smoothed, version. We can then compute the leading error more easily. We write the regularized kernel in the form $K_h(x) = K(x)s(x/h)$ where $s(x) \rightarrow 1$ rapidly as $x \rightarrow \infty$ and s is chosen so that K_h is smooth for all x . Because K is homogeneous, we have $K_h(x) = h^m K_1(x/h)$. For example, if $K(x) = |x|^{-2}$, we could take $K_h(x) = |x|^{-2}(1 - \exp(-|x|^2/h^2))$. Replacing K with K_h introduces an error due to smoothing, but this error can be made higher order in h by imposing moment conditions on s . Now with

$$I = \int_{\mathbb{R}^d} K_h(x)f(x) dx, \quad S = \sum_n K_h(nh)f(nh) h^d \quad (11)$$

we can show that the same error expansion (10) holds. Moreover, because K_1 is regular, the new constant c_0 can be identified using the Poisson Summation Formula:

$$c_0 = (2\pi)^{d/2} \sum_{n \neq 0} \hat{K}_1(2\pi n). \quad (12)$$

We wish to choose K_1 , or s , so that $\hat{K}_1(k)$ decays rapidly for large k , so that only a few terms need to be computed. Of course, we need to know \hat{K}_1 explicitly.

We now return to the question of computing the single layer potential on a surface S . Suppose S is described by coordinates $\alpha = (\alpha_1, \alpha_2)$, so that the points on S are given as $x = x(\alpha)$. We want to use values of the integrand at points regularly spaced in α , so that the points on S are $x_j = x(jh)$. Assume for convenience that the singularity is at $\alpha = 0$, $x(0) = 0$, and the integral extends over $\alpha \in \mathbf{R}^2$. The kernel for the single layer potential is now $K(\alpha) = G(x(\alpha))$, which is approximately $G(J\alpha)$ for $\alpha \approx 0$, where J is the Jacobian matrix $\partial x / \partial \alpha$ at $\alpha = 0$. Thus $1/|x| \approx 1/\sqrt{g_{ij}\alpha_i\alpha_j}$. The constant c_0 will vary with the location of the singularity; it does not appear practical to compute it without modifying the kernel.

We now replace the free space Green's function G with a regular version $G_h(x) = G(x)s(x/h)$, with a radial function s which we choose for our purposes. Then the kernel $G_h(x(\alpha))$ for the modified single layer potential is approximately $G(J\alpha)s(J\alpha/h)$, which has the general form described above, except that it is a function of α rather than x . Consequently we find that

$$\int_{\mathbf{R}^2} G_h(x(\alpha))f(\alpha) d\alpha = \sum_n G_h(x(nh))f(nh)h^2 - c_0f(0)h + O(h^3) \quad (13)$$

with

$$c_0 = 2\pi \sum_{n \neq 0} (G_1 \circ J)^{\wedge}(2\pi n) = 2\pi (\det g^{ij})^{1/2} \sum_{n \neq 0} \Gamma(2\pi \sqrt{g^{ij}n_i n_j}), \quad (14)$$

$$\Gamma(k) = (2\pi)^{-1/2} \int_{-\infty}^{\infty} \hat{G}_1(k, 0, \ell) d\ell. \quad (15)$$

In [4] we use the specific choice of the regularized G ,

$$G_h(x) = -(4\pi|x|)^{-1} (\operatorname{erf}(\rho) + 2\pi^{-1/2}\rho \exp(-\rho^2)), \quad \rho = |x|/h \quad (16)$$

where erf is the error function. This choice has several desirable properties: G_h is smooth and very close to G for x/h large. The smoothing error (the error in the integral because of replacing G with G_h) is $O(h^3)$. Both G_h and Γ can be computed explicitly. Γ decays rapidly, so that the infinite sum (14) can be computed with only a few terms. A further property will be important later; $\hat{G}_h(k) < 0$ for all k , just as $\hat{G}(k) < 0$.

2. Numerical methods for water waves. Next we describe briefly the equations of motion for water waves and the connection with layer potentials in numerical methods. In the usual model of water waves, the fluid is governed by the Euler equations, with the motion assumed incompressible and without viscosity. The upper surface or interface is a free boundary; its location is one of the unknowns. We also assume, as usual, that the motion is irrotational, so that the fluid velocity v satisfies $\nabla \times v = 0$. This, together with the incompressibility condition $\nabla \cdot v = 0$, means that v has the form $v = \nabla \phi$ for a scalar velocity potential ϕ , with $\Delta \phi = 0$ in the fluid region. There are two boundary conditions at the interface: the points move with the fluid velocity; and the pressure p

is zero (neglecting surface tension) to match the atmosphere above. We will suppose the interface is written as $x = x(\alpha, t)$ with coordinates $\alpha = (\alpha_1, \alpha_2)$, and we will consider ϕ on the surface as a function $\phi(\alpha, t)$. The evolution equations on the interface are

$$x_t = v, \quad \phi_t = \frac{1}{2}|v|^2 - gx_3. \quad (17)$$

Here g is the acceleration of gravity, and x_3 is the vertical coordinate. The first equation means that the point with fixed α moves with the fluid velocity, i.e., α_1, α_2 are Lagrangian coordinates. The second equation is a form of Bernoulli's Law, with the pressure set to zero. To complete this set of evolution equations, we need to determine the velocity v at the interface from x and ϕ . This is possible because $\Delta\phi = 0$ in the fluid domain and $v = \nabla\phi$. The tangential gradient of ϕ can be found directly from ϕ on the surface, and so the important part is to determine the normal derivative ϕ_n from ϕ on the surface, given that $\Delta\phi = 0$ in the interior. The operator assigning $\phi \rightarrow \phi_n$ on the surface is called the Dirichlet-to-Neumann operator. Thus the entire fluid motion is determined by what happens on the interface, with Laplace's equation acting as a side condition. The equations have the character of a nonlinear, nonlocal wave equation. Existence results for the exact initial value problem have been difficult to obtain; recent definitive results were given by Sijue Wu [19],[20].

It is helpful to recall the special but important case of the equations linearized at equilibrium. In that case it is convenient to denote the height of the interface at a horizontal point x as $\eta(x, t)$. Then (if the water is infinitely deep) η obeys the equation

$$\eta_{tt} = -g\Lambda\eta \quad (18)$$

where Λ is the operator

$$(\Lambda\eta(\cdot, t))^{\wedge}(k) = |k|\hat{\eta}(k, t). \quad (19)$$

Here $\hat{\eta}$ is the Fourier transform with respect to x , and Λ is the Dirichlet-to-Neumann operator for the half-space. Obviously the wavelike character of the motion depends on the positivity of Λ , and the same is true more generally. It can be seen that the linearization about an *arbitrary* solution of the full water wave equations reduces to an equation for a certain state variable $u(\alpha, t)$ of the form

$$u_{tt} + c\Lambda u \approx 0 \quad (20)$$

where Λ is the principal part of the Dirichlet-to-Neumann operator on the current surface and c is a certain coefficient which is known to be positive. Since $\Lambda \geq 0$, equation (20) is well posed. This structure has implications for the behavior of the numerical method.

Numerical methods for water waves based on the formulation above have been in use for some time, mostly for two-dimensional waves. The methods are of boundary integral type; the velocity is found from layer potentials on the moving interface. Most numerical work has been based on the formulations of Longuet-Higgins and Cokelet [13] and Vinje and Brevig [18]. For recent surveys, see [16],[17]. However, numerical stabilities have often been observed. In [6], T. Hou, J. Lowengrub and the author designed a version of the

method which is numerically stable and convergent. This version is closely related to the work of Baker, Meiron, and Orszag [3]. Recently [4] the author has designed a convergent method in three dimensions, and it is this case that we emphasize here. Another approach in 3D has been given in [12].

In principle, numerical methods based on integrals are too expensive, since with N points, there are N operations needed for each of N integrals, resulting in N^2 operations. However, the operation count can be reduced almost to $O(N)$ using a rapid summation method; see [10] for a recent description of the fast multipole method in 3D. This important development makes numerical methods practical which not be otherwise.

We will not explain the numerical method of [4] here, but rather make some general remarks. In proving convergence of numerical methods for time-dependent problems, we follow a usual outline: We compare the exact problem, in the form $u_t = F(u)$, with a discrete version $u_t^h = F^h(u^h)$. To estimate the growth of $u^h - u$ we add and subtract to get

$$(u^h - u)_t = [F^h(u^h) - F^h(u)] + [F^h(u) - F(u)] \quad (21)$$

or, with $\delta u = u^h - u$.

$$(\delta u)_t \approx dF^h(u)(\delta u) + [F^h(u) - F(u)] \quad (22)$$

The second term on the right in (22) is the consistency error, while the first term has to do with stability. The first term gives us a linear evolution equation which must have bounded growth, independent of h , in order for the method to have numerical stability and converge to the actual solution. For the water wave case, this linear stability equation amounts to a discrete version of (20). Thus it is of primary importance for the discrete form of Λ to be positive. It can be seen that the main part of this discrete Λ is a sum approximating a single layer potential, and thus the choice of quadrature discussed before is critical for the numerical stability.

3. Discrete Boundary Integral Operators. As noted above, the numerical stability of the method for computing water waves depends on the properties of the discrete operators approximating the single layer potential. We assume the surface is doubly periodic. It is convenient to estimate the operators acting on discrete Sobolev spaces. The needed properties are analogues of standard mapping properties of the layer potentials in Sobolev spaces. It is helpful to view the layer potentials as pseudodifferential operators. In [4] we develop some basic properties of discrete pseudodifferential operators; another version of such properties was given in [15]. Since we work with doubly periodic functions of α , it is convenient to use the discrete Fourier transform of a function f on the α -grid. We denote the transform by $\check{f}(k)$; it has period $2\pi/h$ in $k = k_1, k_2$:

$$\check{f}(k) = (2\pi)^{-2} \sum_{j \in I} f(jh) e^{-ikjh} h^2, \quad f(jh) = \sum_{k \in I} \check{f}(k) e^{ikjh} \quad (23)$$

where I is the index set for a fundamental period.

The single layer potential, written as an integral in α , is

$$\int_S G^\pi(x(\alpha) - x(\alpha')) f(\alpha') d\alpha' \quad (24)$$

where we integrate over one period, and G^π means the periodic Green's function. This operator gains one derivative; i.e. it is bounded from H^s to H^{s+1} , where H^s is the Sobolev space of periodic functions with s derivatives in L^2 . The discrete operator, applied to a grid function f , is

$$(Af)_j \equiv \sum_{\ell \in I} G_h^\pi(x_j - x_\ell) f_\ell h^2 \quad (25)$$

where $x_j = x(\alpha_j)$, $\alpha_j = jh$, etc. It is proved in [4], §5, that A gains one discrete derivative, in the sense that AD_h is bounded on discrete L^2 , where D_h is any discrete first order derivative. Furthermore, the principal part of $-A$ has a positivity property explained below, provided $\hat{G}_h(k) < 0$; we saw in §1 that this sign condition on the Fourier transform of G_h could be achieved. As discussed in §2, the positivity property of $-A$ is important for the stability of the numerical method.

To see where these facts come from, we can approximate $x_j - x_\ell$ by $J(\alpha_j)(\alpha_j - \alpha_\ell)$, as in §1. Also, let G_h^0 be the part of G_h near the singularity, cut-off and made periodic, so that $G_h^\pi - G_h^0$ is smooth. Then the important part of A should be

$$(A^{(0)}f)_j \equiv \sum_{\ell \in I} G_h^0(J(\alpha_j)(\alpha_j - \alpha_\ell)) f_\ell h^2. \quad (26)$$

For fixed j we can regard this as a discrete convolution, evaluated at j , of the form

$$(A^{(0)}f)_j = \sum_{\ell \in I} K(jh, jh - \ell h) f_\ell h^2. \quad (27)$$

We can now rewrite this in the discrete transform as

$$(A^{(0)}f)_j = \sum_{k \in I} \check{K}(jh, k) e^{ikjh} \check{f}(k) \quad (28)$$

and we can see from the Poisson Summation Formula that

$$\check{K}(jh, k) = (2\pi)^{-1} \sum_{n \in \mathbb{Z}^2} \hat{K}(jh, k + 2\pi n/h). \quad (29)$$

Here $K(\cdot, jh) = G_h^0 \circ J(\alpha_j)$, so that \hat{K} is related to \hat{G}_h , as in §1.

The operator $A^{(0)}$ of (27), expressed as in (28), looks like a discrete version of a pseudodifferential operator. The standard form is

$$(Tf)(x) = \int a(x, k) e^{ikx} \hat{f}(k) dk \quad (30)$$

and the corresponding discrete form is

$$(Tf)_j = \sum_{k \in I} a(jh, k; h) e^{ikjh} \tilde{f}(k) \quad (31)$$

These discrete operators have properties of boundedness, composition, and positivity like those of the usual ones, but the properties are more restricted unless we assume the operator is cut off for large k ; cf. [15]. There is a form of Gårding's inequality, saying that the operator is essentially positive on discrete L^2 if the symbol $a(jh, k; h)$ is positive. (See §4 of [4].) From (28),(29), the symbol of $-A^{(0)}$ is essentially positive, provided we assume $\hat{G}_h < 0$. Using this fact and estimates for \hat{G}_h , we show ([4], §5) that the operator A of (25) has the form $A = -A^{(1)} - A^{(2)}$, where $A^{(1)}$ is positive, with a gain of one derivative, and $A^{(2)}$ has a gain of two. Since $A^{(1)}$ is the main part of A , its positivity gives the critical property that was needed for the numerical stability as described before.

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